

### AMENDMENTS TO THE CLAIMS

1. (Currently Amended) A computer implemented method~~molecular stereochemical coding, carried out by executing a computer program containing program instructions executable by a computer, for linearly coding molecules, each molecule represented as a stereochemical arrangement of a plurality of atoms, and causing said computer to take a stereochemistry about each of a plurality of atoms constituting a molecule to code the molecule and comparing molecules based on the respective linear code, said instructions method~~ comprising:

classifying atoms of a molecule in a hierarchy by

assigning a start atom to a zero-th hierarchical level as the lowest hierarchy,

assigning all atoms which are directly bonded to said start atom to a first hierarchical level,

assigning all atoms, except said start atom, which are bonded to said atoms assigned to said first hierarchical level, to a second hierarchical level, and similarly,

sequentially assigning atoms to hierarchical levels until a final hierarchy is made based on all atoms of said molecule~~in a form which may be accessed by a processor;~~

forming a molecular tree ~~with a precedence rule~~ by placing said atoms, which belong to the same hierarchical level, in an order, ~~in accordance with said precedence rule to form said molecular tree wherein said start atom from a lower hierarchical level~~ having said start atom to a higher hierarchical level is expressed in a bonding relationship between said plurality of atoms of said molecule;

coding one atom, which was assigned to ~~a~~ the (n+3)-th hierarchical level, wherein n is an integer of 0 or more, in said molecular tree, by

deriving a dihedral angle between a theoretical plane, which is formed by an atom in the (n+3)-th hierarchical level, an atom in ~~a~~ the (n+2)-th hierarchical level and an atom in ~~a~~ the (n+1)-th hierarchical level, and a theoretical plane, which is formed by the atom in the (n+2)-th hierarchical level, the atom in the (n+1)-th hierarchical level and an atom in ~~a~~ the n-th hierarchical level, with respect to a group comprising four atoms which consists of said coded atom in the (n+3)-th hierarchical level, the atom in the (n+2)-th hierarchical level which is bonded to the atom in the (n+3)-th hierarchical level, the atom in the (n+1)-th hierarchical level which is bonded to the atom in the (n+2)-th hierarchical level, and the atom in the n-th hierarchical level which is bonded to the atom in the (n+1)-th hierarchical level,

replacing the derived dihedral angle with an angular symbol ~~in accordance with an angle dividing rule (ADR)~~ based on the magnitude of the dihedral angle,

assigning the angular symbol to the coded atom in the (n+3)-th hierarchical level, and

similarly, assigning angular symbols based on the magnitudes of dihedral angles with respect to other atoms to be coded;

~~with a linear notation rule, expressing said molecular tree in a linear notation coded by a row of characters, carrying out linear notation of a set of said angular symbols in accordance with said linear notation rule so as to correspond to said molecular tree;~~

preparing a conformation code which is indicative of a conformation of the molecule with respect to said start atom, ~~and;~~ similarly,

preparing conformation codes ~~with respect to~~ using others of said plurality of atoms of said molecule as other start atoms; and

storing said conformation codes for said molecule in a memory of said computer; and

comparing said conformation codes for said molecule with stored conformation codes of at least one other of said molecules in order to determine if molecules, or regions of molecules, have the same conformation

~~further comprising printing or recording the conformation code of the molecule on computer readable recording media.~~

2. (Currently Amended) The computer implemented method~~program~~ as set forth in claim 1, ~~which further comprises instructions for~~ further comprising,

after said preparing and storing conformation codes for said molecule, preparing  
a configuration code indicative of a configuration of the molecule ~~for~~ with respect  
to said start atom, and including

coding an atom in the n-th hierarchical level by

assigning said atom as a reference position,

integrally rotating all of the atoms belonging to the (n+3)-th  
hierarchical level around a bonding axis, which connects the atom in the  
(n+1)-th hierarchical level to the atom in the (n+2)-th hierarchical level, so  
that an atom, which has precedence ~~in accordance with said precedence~~  
~~rule~~ among said atoms belonging to the (n+3)-th hierarchical level, is  
positioned at an angular position with respect to said reference position,

~~giving~~ assigning an angular symbol ~~according to said ADR~~ to each of  
said atoms belonging to the (n+3)-th hierarchical level, in accordance with  
an angular position after rotation with respect to said reference position,

carrying out the linear notation of a set of said plurality of angular  
symbols ~~in accordance with said linear notation rule so as to correspond to~~  
in correspondence with said molecular tree, ~~and~~

preparing a configuration code which is indicative of a configuration  
of the molecule with respect to ~~for~~ said start atom,

similarly, preparing configuration codes using others of said plurality  
of atoms of said molecule as start atoms, and

storing said configuration codes for said molecule in a memory of said computer.

3. (Currently Amended) The computer ~~implemented method~~program as set forth in claim 1 ~~or 2, which further comprises instructions for further comprising,~~ after preparing and storing conformation codes and configuration codes for said molecule, preparing a planar structure code indicative of a planar structure of the molecule ~~for~~with respect to said start atom, wherein said molecular tree is expressed by a set of planar structure symbols which planar-structurally express a bonding relationship between said plurality of atoms, said preparing a planar structure code including

carrying out the linear notation of said set of planar structure symbols ~~in accordance with said linear notation rule so as to correspond to in~~ correspondence with said molecular tree,

preparing a planar structure code indicative of the planar structure of the molecule with respect to said start atom, ~~and~~

similarly, preparing planar structure codes ~~with respect to other~~ using others of said plurality of atoms of said molecule as start atoms, and

storing said planar structure codes for said molecule in a memory of said computer.

4. (Currently Amended) The computer implemented method~~program~~ as set forth in claim 3, wherein said conformation codes, said configuration codes and said planar structure codes are expressed ~~in parallel~~ beginning with respect to said start atoms.

5. (Currently Amended) The computer implemented method~~program~~ as set forth in claim 2, wherein when it is substantially impossible to rotate said atoms belonging to the (n+3)-th hierarchical level around the bonding axis connecting the atom belonging to the (n+1)-th hierarchical level to the atom belonging to the (n+2)-th hierarchical level, said angular symbols given at said coding step are adopted as they are, and the linear notation of a set of said plurality of angular symbols is carried out ~~in accordance with said linear notation rule~~ so as to correspond to said molecular tree, to prepare said configuration codes for said start atom.

6. (Canceled).

7. (Canceled).

8. (Currently Amended) The computer implemented method~~program~~ as set forth in claim 1, wherein said ~~linear notation rule~~ linear notation coded by the set of said angular symbols is based on a CANOST code linear notation rule, said

CANOST code linear notation being a linear list of symbols which express the bonding relationship between a plurality of atoms.

9. (Currently Amended) The computer implemented method~~program~~ as set forth in claim 1, wherein during the formation of said molecular tree, a group of atoms ~~having a low degree of coding in the identification of stereochemistry~~ are replaced with symbols to be masked.

10. (Currently Amended) The computer implemented method~~program~~ as set forth in claim 1, wherein said ~~ADR~~ replacing said dihedral angle with an angular symbol includes dividing~~divides~~ an angle of 360 degrees into a number of clock-dial-like angular ranges, ~~and the divided angular ranges are reflected in the level of abundance to be unequally divided.~~

11. (Currently Amended) The computer implemented method~~program~~ as set forth in claim 1, wherein during the preparation of said conformation codes, said conformation codes are prepared with respect to at least two of said start atoms, the hierarchical ~~level numbers~~ levels of which are spaced from each other by three hierarchical levels or more.

12. (Cancelled).

13. (Currently Amended) A computer readable storage medium containing instructions, executed by a processor, for performing a method for ~~taking a stereochemistry about each of a plurality of atoms constituting a molecule to code the molecule~~linearly coding molecules, each molecule represented as a stereochemical arrangement of a plurality of atoms, and comparing molecules based on the respective linear code, said method comprising:

classifying atoms of a molecule in a hierarchy by

assigning a start atom to a zero-th hierarchical level as the lowest hierarchy,

assigning all atoms which are directly bonded to said start atom to a first hierarchical level,

assigning all atoms, except said start atom, which are bonded to said atoms assigned to said first hierarchical level, to a second hierarchical level, and similarly, and

sequentially assigning atoms to hierarchical levels until a final hierarchy is made based on all atoms of said molecule ~~in a form which may be accessed;~~

forming a molecular tree ~~with a precedence rule~~ by placing said atoms, which belong to the same hierarchical level, in an order, ~~in accordance with said precedence rule to form a molecular tree wherein said start atom from a lower~~



hierarchical level having said start atom to a higher hierarchical level is expressed in a bonding relationship between said plurality of atoms of said molecule;

coding one atom, which was assigned to a the (n+3)-th hierarchical level, wherein n is an integer of 0 or more, in said molecular tree, by

deriving a dihedral angle between a theoretical plane, which is formed by an atom in the (n+3)-th hierarchical level, an atom in a the (n+2)-th hierarchical level and an atom in a the (n+1)-th hierarchical level, and a theoretical plane, which is formed by the atom in the (n+2)-th hierarchical level, the atom in the (n+1)-th hierarchical level and an atom in a the n-th hierarchical level, with respect to a group comprising four atoms which consists of said coded atom in the (n+3)-th hierarchical level, the atom in the (n+2)-th hierarchical level which is bonded to the atom in the (n+3)-th hierarchical level, the atom in the (n+1)-th hierarchical level which is bonded to the atom in the (n+2)-th hierarchical level, and the atom in the n-th hierarchical level which is bonded to the atom in the (n+1)-th hierarchical level,

replacing the derived dihedral angle with an angular symbol ~~in accordance with an angle dividing rule (ADR)~~ based on the magnitude of the dihedral angle,

assigning the angular symbol to the coded atom in the (n+3)-th hierarchical level, and

similarly, assigning angular symbols based on the magnitudes of dihedral angles with respect to other atoms to be coded; ~~and~~

~~with a linear notation rule, expressing said molecular tree in a linear notation coded by~~ by a row of characters, carrying out linear notation of a set of said angular symbols in accordance with said linear notation rule so as to correspond to said molecular tree;

preparing a conformation code which is indicative of a conformation of the molecule with respect to said start atom, ~~and;~~

similarly, preparing conformation codes ~~with respect to other~~ using others of said plurality of atoms of said molecule as start atoms;

storing said conformation codes for said molecule in a memory of said computer; and

comparing said conformation codes for said molecule with said stored conformation codes of at least one other of said molecules in order to determine if molecules have the same conformation

~~wherein the codes of the molecule are recorded in a computer readable recording medium to give the stereochemistry about each of a plurality of atoms constituting the molecule.~~

14. (Currently Amended) The computer implemented method~~program~~ as set forth in claim ~~13~~, further comprising calculating ~~predicting~~ NMR shifts based

upon said conformation codes, said configuration codes, or said planar codes, or combinations thereof.

15. (Currently Amended) The computer implemented method~~program~~ as set forth in claim 14, ~~wherein~~ further comprising recording the NMR shifts are printed on computer readable recording media.

16. (Currently Amended) The computer implemented method~~program~~ as set forth in claim 2, further comprising ~~printing or~~ recording the configuration code of the molecule on computer readable recording media.

17. (Cancelled).

18. (Currently Amended) A computer, including a computer program containing program instructions executed by said computer, method for taking a stereochemistry about each of a plurality of atoms constituting a molecule to code the molecule linearly coding molecules, each molecule represented as a stereochemical arrangement of a plurality of atoms, and comparing molecules based on the respective linear code, said computer~~method~~ comprising:

classifying atoms of a molecule in a hierarchy by

assigning a start atom to a zero-th hierarchical level as the lowest hierarchy,

assigning all atoms which are directly bonded to said start atom to a first hierarchical level,

assigning all atoms, except said start atom, which are bonded to said atoms assigned to said first hierarchical level, to a second hierarchical level, and similarly,

sequentially assigning atoms to hierarchical levels until a final hierarchy is made based on all atoms of said molecule ~~in a form which may be accessed~~;

forming a molecular tree ~~with a precedence rule~~ by placing said atoms, which belong to the same hierarchical level, in an order, ~~in accordance with said precedence rule to form a molecular tree wherein said start atom from a lower hierarchical level~~ having said start atom to a higher hierarchical level is expressed in a bonding relationship between said plurality of atoms of said molecule;

coding one atom, which was assigned to a ~~the~~ (n+3)-th hierarchical level, wherein n is an integer of 0 or more, in said molecular tree, by

deriving a dihedral angle between a theoretical plane, which is formed by an atom in the (n+3)-th hierarchical level, an atom in a ~~the~~ (n+2)-th hierarchical level and an atom in a ~~the~~ (n+1)-th hierarchical level, and a plane, which is formed by the atom in the (n+2)-th hierarchical level, the atom in the (n+1)-th hierarchical level and an atom in a ~~the~~ n-th hierarchical level, with respect to a group comprising four atoms which consists of said coded atom in the (n+3)-th hierarchical level, the atom in

the (n+2)-th hierarchical level which is bonded to the atom in the (n+3)-th hierarchical level, the atom in the (n+1)-th hierarchical level which is bonded to the atom in the (n+2)-th hierarchical level, and the atom in the n-th hierarchical level which is bonded to the atom in the (n+1)-th hierarchical level,

replacing the derived dihedral angle with an angular symbol ~~in accordance with an angle dividing rule ADR~~ based on the magnitude of the dihedral angle,

assigning the angular symbol to the coded atom in the (n+3)-th hierarchical level, and

similarly, assigning angular symbols based on the magnitudes of dihedral angles with respect to other atoms to be coded; ~~and~~

~~with a linear notation rule, expressing said molecular tree in a linear notation coded by~~ by a row of characters, carrying out linear notation of a set of said angular symbols in accordance with said linear notation rule so as to correspond to said molecular tree;

preparing a conformation code which is indicative of a conformation of the molecule with respect to said start atom, and similarly;

preparing conformation codes ~~with respect to~~ using others of said plurality of atoms of said molecule as other start atoms;

storing said conformation codes for said molecule in a memory of said computer; and

comparing said conformation codes for said molecule with stored conformation codes of at least one other of said molecules in order to determine if molecules have the same conformation.

19. (New) The computer implemented method as set forth in claim 1, wherein said molecules are organic molecules, and said comparing compares conformation codes for one organic molecule with stored conformation codes of at least one other of said organic molecules in order to determine if the organic molecules, or regions of the organic molecules, have the same conformation.

20. (New) The computer implemented method as set forth in claim 1, wherein said molecules are molecules of Sugar, and said comparing compares conformation codes for a Sugar molecule with stored conformation codes of at least one other of said Sugar molecules in order to determine if the Sugar molecules, or regions of the Sugar molecules, have the same conformation.